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Pair Interaction in a Transition-Metal Nano State

Nikolay Dubinin[1,2]

[1)] Ural Federal University, Mira st. 19, 620002 Ekaterinburg, Russia
[2)] Institute of Metallurgy of the Ural Branch of the Russian Academy of Sciences, Amundsen st. 101, 620016 Ekaterinburg, Russia
ned67@mail.ru

Abstract

It is found that the depth of the first minimum of the Wills-Harrison effective pair potential and oscillations of its long-range part increase at transition from liquid to nano state in both Fe and Ni.

Keywords: Transition metal, Wills-Harrison model, nano state

The Wills-Harrison (WH) model [1] is used to study the transition-metal pair interactions in the nano state.

The WH effective pair potential is

$$\varphi_{\mathrm{WH}}(r) = \varphi_s(r) + \varphi_d(r) \quad , \tag{1}$$

where $\varphi_s(r)$ and $\varphi_d(r)$ are the contributions due to the *s*- and *d*-electron states, respectively. The first is taken here in the framework of the Bretonnet-Silbert (BS) model [2]. The second is expressed as follows (in a.u.):

$$\varphi_d(r) = -z_d\left(\frac{10 - z_d}{10}\right)\left(\frac{12}{\nu}\right)^{1/2} \frac{r_d^3}{r^5} K_b + z_d \frac{r_d^6}{r^8} K_c \quad , \tag{2}$$

where z_d is the effective *d*-electron valence, r_d - *d*-state radius, K_b and K_c - combinatoric coefficients, ν - coordination number.

We take into consideration Fe and Ni in liquid and nano states. The WH and BS input parameters are taken from [1] and [3]. The coordination number is taken equal to 12 for both metals. The experimental values of the mean atomic volume, Ω, equal to 89.29 a.u. for liquid Fe and equal to 85.24 a.u. for liquid Ni are taken from [4]. For the nano state values of Ω have been calculated from the values named above as 68.69 a.u. and 65.57 a.u. for Fe and Ni, respectively.

Figs. 1, 2 show that the depth of the first minimum of $\varphi_{\mathrm{WH}}(r)$ and

oscillations of its long-range part become more considerable in the nano state. The first tendency is more inherent in Fe and the second, on the contrary, in Ni.

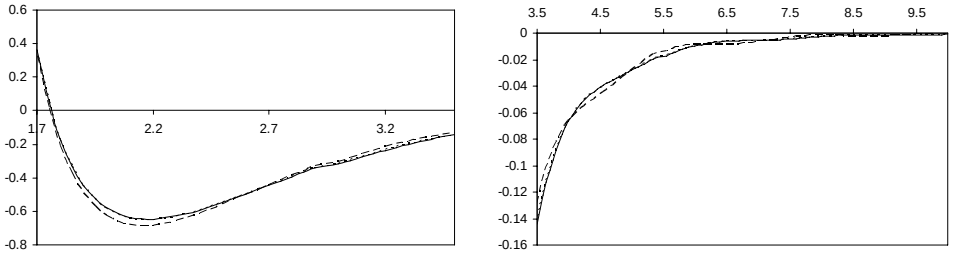

Figure 1. Short- and long-range parts of $\varphi_{\mathrm{WH}}(r)$ (eV) in Fe (liquid state - solid line; nano state - dashed line).

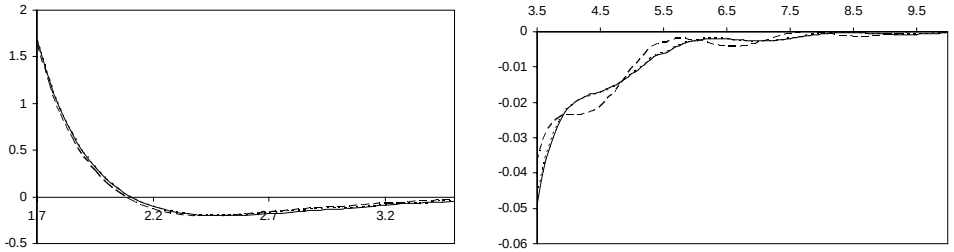

Figure 2. Short- and long-range parts of $\varphi_{\mathrm{WH}}(r)$ (eV) in Ni (liquid state - solid line; nano state - dashed line).

Acknowledgments

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